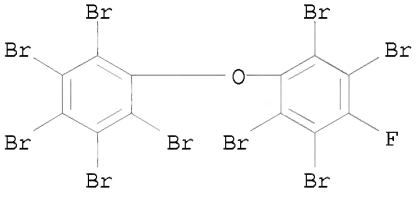
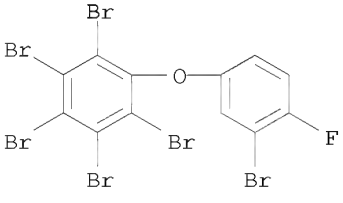
L2 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2010 ACS on STN
RN 876310-29-1 REGISTRY
ED Entered STN: 09 Mar 2006
CN Benzene, 1,2,3,4,5-pentabromo-6-(2,3,5,6-tetrabromo-4-fluorophenoxy)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, pentabromo(2,3,5,6-tetrabromo-4-fluorophenoxy)- (9CI)
OTHER NAMES:
CN 4'-Fluoro-2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether
MF C12 Br9 F O
SR CA
LC STN Files: CA, CAPLUS, CHEMCATS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2010 ACS on STN
RN 863314-88-9 REGISTRY
ED Entered STN: 16 Sep 2005
CN Benzene, 1,2,3,4,5-pentabromo-6-(3-bromo-4-fluorophenoxy)- (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzene, pentabromo(3-bromo-4-fluorophenoxy)- (9CI)
OTHER NAMES:
CN 4'-Fluoro-2,3,3',4,5,6-hexabromodiphenyl ether
MF C12 H3 Br6 F O
SR CA
LC STN Files: CA, CAPLUS, CHEMCATS, CSCHEM, TOXCENTER, USPATFULL



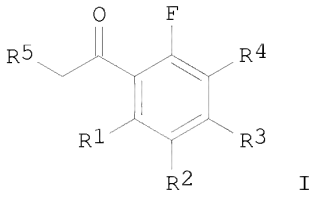
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

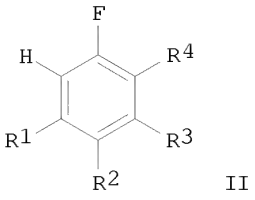
```
=> fil caplus
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       196.23     196.45

FILE 'CAPLUS' ENTERED AT 14:15:37 ON 17 JUL 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2010 AMERICAN CHEMICAL SOCIETY (ACS)
```



```
FILE COVERS 1907 - 17 Jul 2010  VOL 153 ISS 4
FILE LAST UPDATED: 16 Jul 2010  (20100716/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Apr 2010

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l2
L3            6 L2

=> d 1-6 bib abs hitstr

L3   ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2010 ACS on STN
AN   2009:791044  CAPLUS
DN   151:100911
TI   Preparation of acetophenone derivatives by ortho-lithiation of substituted
     fluorobenzenes
IN   Obitsu, Kazuyoshi; Kimura, Takenori
PA   Astellas Pharma Inc., Japan
SO   Jpn. Kokai Tokkyo Koho, 12pp.
     CODEN: JKXXAF
DT   Patent
LA   Japanese
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ---------------     ----   --------    --------------------   --------
PI   JP 2009143885        A     20090702    JP 2007-325911         20071218
PRAI JP 2007-325911               20071218
OS   MARPAT 151:100911
GI
```



I



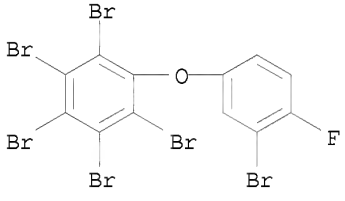
II

AB Acetophenone derivs. I [R1-R3 = H, cyano, A-O, A-S, A-CO, A'-O-A (A = lower alkyl; A' = lower alkylene), protected carboxyl, (un)substituted aryl(oxy); R4 = H, halo, lower alkyl; R5 = halo, lower alkyl], useful for drug intermediates, are prepared by reacting II (R1-R4 = the same as above) with reaction equivalent amount of bulky and weakly nucleophilic strong bases and then with reaction equivalent amount of N-lower-alkoxy-N-lower alkylamide derivs. R5CH2CONR6OR7 (R6, R7 = lower alkyl) in inert solvents. Thus, diisopropylamine was reacted with n-BuLi and 1-bromo-2-fluorobenzene and then with 2-chloro-N-methoxy-N-methylacetamide and purified on silica gel column chromatog. to afford 1-(3-bromo-2-fluorophenyl)-2-chloroethanone in 70.9% yield.

IT 863314-88-9
RL: PRPH (Prophetic); RCT (Reactant); RACT (Reactant or reagent)
(preparation of acetophenone derivs. by ortho-lithiation of substituted fluorobenzenes followed by reaction with predetd. alkylamines)

RN 863314-88-9 CAPLUS

CN Benzene, 1,2,3,4,5-pentabromo-6-(3-bromo-4-fluorophenoxy)- (CA INDEX NAME)



L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN

AN 2008:1410036 CAPLUS

DN 150:135781

TI The determination of polybrominated diphenyl ether congeners by gas chromatography inductively coupled plasma mass spectrometry

AU Swarthout, Robert F., Jr.; Kucklick, John R.; Davis, W. Clay

CS Graduate Program in Environmental Studies, College of Charleston, Charleston, SC, 29424, USA

SO Journal of Analytical Atomic Spectrometry (2008), 23(12), 1575-1580
CODEN: JASPE2; ISSN: 0267-9477

PB Royal Society of Chemistry

DT Journal

LA English

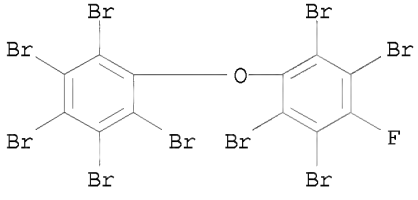
AB Polybrominated di-Ph ethers (PBDE) are flame retardant chems. used in everyday household items such as computer casings and household textiles. Leaching and migration of these chems. from products is reported as the cause for the widespread presence of these compds. in the authors' environment. While PBDEs are predominantly analyzed by GC-NCI-MS,

GC-HRMS, or GC-ECD, this paper studies the potential of GC-ICP-MS for the determination of PBDEs. The application of this methodol. for the anal. of PBDEs in NIST SRM 2977 Mussel Tissue and NIST 1941b Marine Sediment is also presented. The extreme sensitivity of inductively coupled plasma mass spectrometry (ICP-MS) for atomic information makes GC-ICP-MS a promising alternative for analyzing PBDEs at low concns. or in small sample sizes. The instrumental detection limits of a GC-NCI-MS were directly compared to those of a GC-ICP-MS for a mixture of 28 PBDE congeners including the decabrominated PBDE-209 congener. The GC-ICP-MS instrumental method demonstrated superior sensitivity over the GC-NCI-MS for all of the PBDE congeners with absolute detection limits ranging from 0.2 pg to 0.3 pg as compared to 1.5 pg to 24.3 pg for GC-NCI-MS. The GC-ICP-MS method was then used to quantify PBDE congeners in Standard Reference Material (SRM) 1941b Orgs. in Marine Sediment and SRM 2977 Freeze-Dried Mussel Tissue (Organic Contaminants and Trace Elements). The mass fraction of PBDE congeners in these SRMs determined by GC-ICP-MS were within 13% (8.5%) and 7% (2.5%) (mean difference (1 SD)) of previously determined values for SRMs 1941b and 2977, resp. The PBDE 209 value in SRM 1941b determined by GC-ICP-MS compared favorably to the consensus value from a recent interlab. comparison using this material (28.7 ng/g-1 ± 2.9 ng/g-1 vs. 24.4 ng/g-1 ± 14.1 ng/g-1).

IT 876310-29-1, 4'-Fluoro-2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether
RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); ANST (Analytical study); USES (Uses)
(determination of polybrominated di-Ph ether congeners by gas chromatog. inductively coupled plasma mass spectrometry)

RN 876310-29-1 CAPLUS

CN Benzene, 1,2,3,4,5-pentabromo-6-(2,3,5,6-tetrabromo-4-fluorophenoxy)- (CA INDEX NAME)



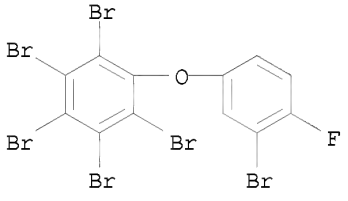
OSC.G 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
AN 2006:556874 CAPLUS
DN 145:254216
TI Synthesis of fluorinated polybrominated diphenyl ethers (F-PBDEs) as internal standards for environmental analysis
AU Liu, Huiling; Skalvoll, Anja; Reijerink, Gaby S.; Luthe, Gregor; Johansen, Jon E.
CS Chiron AS, Trondheim, N-7041, Norway
SO Chemosphere (2006), 64(2), 250-255
CODEN: CMSHAF; ISSN: 0045-6535
PB Elsevier B.V.
DT Journal
LA English
AB Polybrominated di-Ph ethers (PBDE) are widely distributed environmental

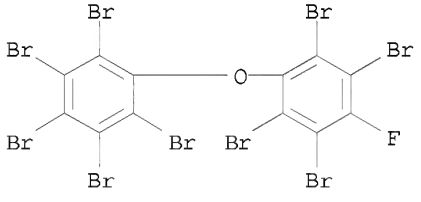
pollutants due to their wide-spread use as flame retardants. Their structural similarity to other halogenated organic pollutants, e.g., polychlorinated biphenyls (PCB), led to speculation they may have similar toxicol. properties and effects. Recent focus on PBDE as possible priority pollutants also led to an increasing need for PBDE reference stds. for toxicol. studies and environmental anal. In this work, a series of fluorinated PBDE (F-PBDE) which can be used as possible internal stds. as an alternative to high-cost alternatives, e.g., 13C-labeled analogs, were synthesized. F-PBDE were synthesized using different coupling reactions and via bromination of fluorinated starting materials.

IT 863314-88-9P, 4'-Fluoro-2,3,3',4,5,6-hexabromodiphenyl ether
876310-29-1P, 4'-Fluoro-2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether
RL: CPS (Chemical process); NUU (Other use, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(synthesis of fluorinated polybrominated di-Ph ethers as internal stds. for brominated di-Ph ether environmental anal.)

RN 863314-88-9 CAPLUS
CN Benzene, 1,2,3,4,5-pentabromo-6-(3-bromo-4-fluorophenoxy)- (CA INDEX NAME)



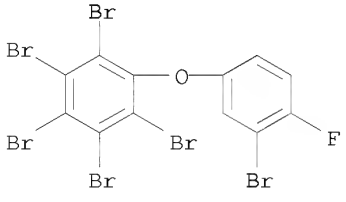
RN 876310-29-1 CAPLUS
CN Benzene, 1,2,3,4,5-pentabromo-6-(2,3,5,6-tetrabromo-4-fluorophenoxy)- (CA INDEX NAME)



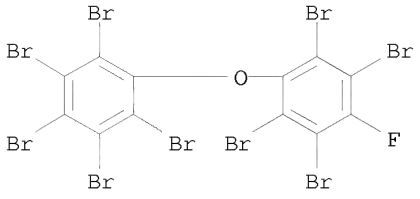
OSC.G 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
AN 2006:287705 CAPLUS
DN 144:500728
TI Monofluorinated analogues of polybrominated diphenyl ethers as analytical standards: synthesis, NMR, and GC-MS characterization and molecular orbital studies
AU Luthe, Gregor; Leonards, Pim E. G.; Reijerink, Gaby S.; Liu, Huling; Johansen, Jon E.; Robertson, Larry W.

CS Institute of Chemistry, Norwegian University of Science and Technology, Trondheim, N-7041, Norway
SO Environmental Science & Technology (2006), 40(9), 3023-3029
CODEN: ESTHAG; ISSN: 0013-936X
PB American Chemical Society
DT Journal
LA English
AB Polybrominated di-Ph ethers (PBDEs), a group of 209 individual congeners distinguishable by the number and position of bromines, are produced for use as flame retardants in consumer goods. PBDEs have become ubiquitous environmental contaminants, present in increasing levels in the environment and humans. Ten individual monofluorinated analogs of PBDEs (F-PBDEs) and one difluorinated PBDE (FF-PBDE) were synthesized and characterized, and their gas chromatog. (GC) and mass spectrometric (MS) characteristics determined The synthesis method used a nucleophilic reaction of bromophenols with diphenyliodonium salts and the perbromination of fluorosubstituted di-Ph ethers. Reaction yields were 10-59% with ≥98% purity. Apart from the aromatic ring carrying the fluorine atom, only minor chemical NMR shift changes were observed in comparison to the corresponding parent PBDEs, with the exception that the JF,H coupling was stronger. The authors' preliminary data show that F-PBDEs and PBDEs have comparable retention times in gas chromatog. with F-PBDEs demonstrating in general shorter or identical retention times, depending on the pattern of fluorine substitution. The authors also calculated the torsion angles and the dipole moments for both and report that there is a good correlation between GC retention times and the torsion angles but not with dipole moments. In MS, the difference of the ion peaks of the F-PBDE/PBDE pairs is m/z 19 (F), which allows a simultaneous MS detection without separation From GC separation, simultaneous MS detection, and the stability of fluorine due to its generally resistance to nucleophilic displacement, probably F-PBDEs functions as valuable potential stds., markers, and tracers in environmental anal.
IT 863314-88-9P 876310-29-1P
RL: ARU (Analytical role, unclassified); NUU (Other use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)
(synthesis, NMR, and GC-MS characterization and MO studies of monofluorinated analogs of polybrominated di-Ph ethers as anal. stds. in polybrominated di-Ph ether anal.)
RN 863314-88-9 CAPLUS
CN Benzene, 1,2,3,4,5-pentabromo-6-(3-bromo-4-fluorophenoxy)- (CA INDEX NAME)



RN 876310-29-1 CAPLUS
CN Benzene, 1,2,3,4,5-pentabromo-6-(2,3,5,6-tetrabromo-4-fluorophenoxy)- (CA INDEX NAME)



OSC.G 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)
RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN
AN 2005:902834 CAPLUS
DN 143:248154
TI Preparation of congeneric, chlorinated, brominated and/or iodinated, fluorinated aromatic compounds comprising two benzene rings in their structure.
IN Liu, Huiling; Luthe, Gregor; Johansen, Jon Eigill
PA Chiron A/S, Norway
SO PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005077868	A2	20050825	WO 2005-EP50779	20050216
	WO 2005077868	A3	20060511		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 102004007358	A1	20050901	DE 2004-102004007358	20040216
	US 20070298501	A1	20071227	US 2007-589597	20070530
PRAI	DE 2004-102004007358	A	20040216		
	WO 2005-EP50779	W	20050216		

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OS MARPAT 143:248154
GI

I

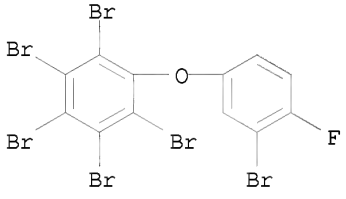
AB Title compds., e.g. [A1LpB1, I; p = 0, 1; A1 = monovalent monofluorinated Ph, monovalent chlorinated, brominated, and/or iodinated, monofluorinated Ph; B1 = monovalent chlorinated, brominated and/or iodophenyl or monovalent unhalogenated Ph; A2 = divalent monofluorinated Ph, divalent

chlorinated, brominated and/or iodinated, monofluorinated Ph; B2 = divalent chlorinated, brominated and/or iodinated Ph or divalent nonhalogenated Ph; L = O, S, alkylene; with provisos], were prepared Thus, 2,4-dibromophenol, 3,3'-dibromo-4,4'-difluorophenyliodonium chloride (preparation given) and NaOH were refluxed together in H2O for 15 min. to give 59.3% 4'-fluoro-2,3',4-tribromodiphenyl ether.

IT 863314-88-9P
RL: ARU (Analytical role, unclassified); BSU (Biological study, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation)
(claimed compound; preparation of congeneric, chlorinated, brominated and/or iodinated, fluorinated aromatic compds. comprising 2 benzene rings in their structure)

RN 863314-88-9 CAPLUS

CN Benzene, 1,2,3,4,5-pentabromo-6-(3-bromo-4-fluorophenoxy)- (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2010 ACS on STN

AN 2005:701619 CAPLUS

DN 144:246078

TI Monofluorinated analogues of polybrominated diphenylethers (F-PBDEs) - standards for analysis: retention behaviour in gas chromatography

AU Luthe, Gregor; Leonards, Pim E. G.; Liu, Huiling; Johansen, Jon E.

CS Chiron, Trondheim, Norway

SO Organohalogen Compounds (2004), 66(Dioxin 2004), 3666-3672
CODEN: ORCOEP; ISSN: 1026-4892

PB International Symposium on Halogenated Environmental Organic Pollutants and Persistent Organic Pollutants

DT Journal; (computer optical disk)

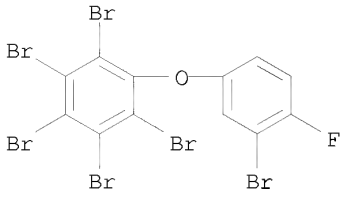
LA English

AB In the present study, the authors focused attention on the retention behavior of monofluorinated polybrominated di-Ph ethers (F-PBDEs) in GC, with the intention to use them as calibration stds. for electron impact mass spectrometry (EI-MS) and GC-MS in the neg. chemical ionisation mode (ECNI) GC-ECNI-MS.

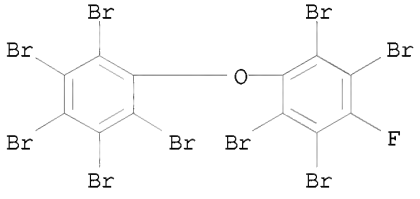
IT 863314-88-9, 4'-Fluoro-2,3,3',4,5,6-hexabromodiphenyl ether
876310-29-1, 4'-Fluoro-2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether
RL: ARU (Analytical role, unclassified); PRP (Properties); ANST (Analytical study)
(monofluorinated analogs of polybrominated diphenylethers as stds. for polybrominated di-Ph ether anal. by GC-MS)

RN 863314-88-9 CAPLUS

CN Benzene, 1,2,3,4,5-pentabromo-6-(3-bromo-4-fluorophenoxy)- (CA INDEX NAME)



RN 876310-29-1 CAPLUS
CN Benzene, 1,2,3,4,5-pentabromo-6-(2,3,5,6-tetrabromo-4-fluorophenoxy)- (CA INDEX NAME)



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>